

CENTRAL EUROPEAN CHEMICAL MEETING (CECM-1)

Varaždin, Croatia

PROGRAM

Wednesday, June 14, 2000

19:00 - 21:00 Registration

Thursday, June 15, 2000

09:00 - 09:30 Opening addresses

CONFERENCE PART

Chairperson: Vitomir Šunjić

09:30 **Istvan Hargittai**, Budapest Technical University, Hungary

Great Chemical Discoveries from a Central European Perspective

10:30 - 11:00 Coffee break

11:00 **Gabor Naray-Szabo**, Lornad Eoetvoes University, Budapest, Hungary

Structure-Based Molecular Design

11:50 **Rudolf Janoschek**, Karl-Franzens-Universitat Graz, Austria

Theoretical Studies on Heterocumulated Double Bond Systems

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Chairperson: Ante Graovac

15:00 **Tibor Braun, Wolfgang Glanzel**, Lorand Eotvoes University, Budapest, Hungary
Information Science and Scientometric Research Unit (ISSRU),
Hungarian Academy of Sciences, Budapest

Chemistry Research in East Central Europe as Reflected in its Journal Literature

15:50 **Doina Bejan**, Technical University Gh. Asachi, Iasi, Romania

Spectrometric Methods. A solution for the Trace Analysis

16:25 **Gergely Dezso**, Department of Theoretical Physics, Szeged University, Szeged, Hungary

On the Construction of Perfectly N-Representable Two-electron Density Matrices for Energy Optimization

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19:00 Alchemy Exposition and Concert

Friday, June 16, 2000

Chairperson: Drazen Vikić-Topic

09:00 **Vitomir Šunjić**, Laboratory of Stereoselective Catalysis and Biocatalysis, Ruđer Bošković Institute, Zagreb, Croatia

Recent Synthetic and Spectroscopic Studies of Some Enantioselective Biocatalytic Reactions

09:50 **Alan Marschand**, Department of Chemistry, University of North Texas, Denton, Texas, USA

Novel Cage-Annulated Crown Ethers, Cryptands, and Molecular Boxes: A New Class of Ionophores for Selective Ion Complexation

10:40 Coffee break

11:00 **Srdanka Tomić-Pisarović**, Laboratory of Organic Chemistry, Department of Chemistry, Faculty of Science, University of Zagreb, Croatia

Selective Hydrolyses Catalyzed by Esterases from Mammalian Sera

11:35 **Olga Kronja**, Faculty of Pharmacy and Biochemistry, University of Zagreb, Croatia

Solvolysis of 1,1-Dimethyl-4-alkenyl Chlorides. Evidence of p-Participation

AFTERNOON TRIP : Varaždinske Toplice and Imbriovec (Dinner will be served)

Saturday, June 17, 2000

Chairperson: Hrvoj Vanik

09:00 **Jure Zupan**, National Institute of Chemistry, Ljubljana, Slovenia

Artificial Neural Network in Chemistry

09:50 **Petr Čarsky**, J. Heyrovsk Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Development of an Approximate Multi-Reference Coupled-Cluster Method

10:40 Coffee break

11:00 **Jerzy Cioslowski**, Department of Chemistry and Supercomputer Computations Research Institute, Florida State University, Tallahassee, FL, U.S.A.

Standard Enthalpies of Formation of IPR Fullerenes and their Analysis in Terms of Structural Motifs

11:50 **Csaszr Attila**, Department of Theoretical Chemistry, Eotvoes University, Budapest, Hungary

Ab initio Rovibrational Spectroscopy

12:40 CLOSING OF THE MEETING